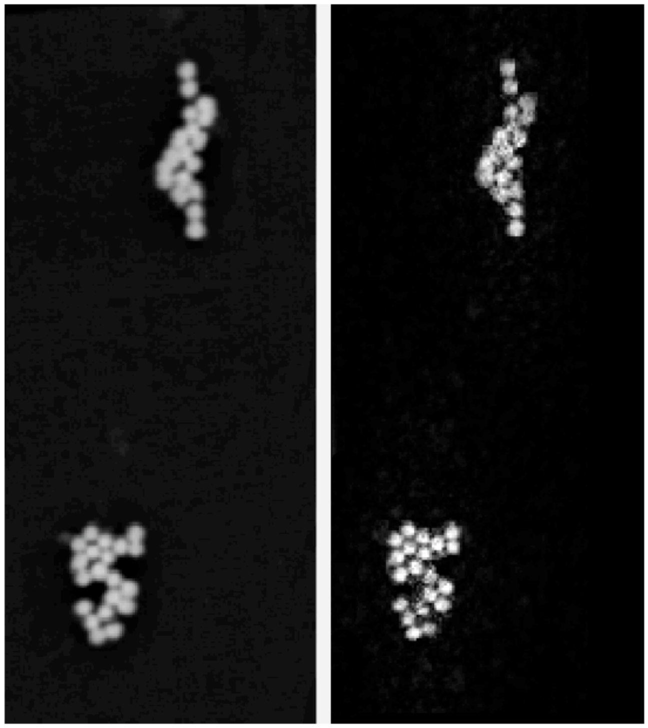
COHERENT X-RAY DIFFRACTIVE IMAGING AT THE ADVANCED LIGHT SOURCE

The rapid growth of nanoscience has produced an urgent need for techniques capable of revealing the internal structure, in three dimensions, of inorganic nanostructures and large molecules which cannot be crystallized (such as the membrane proteins of vital importance for drug delivery). Scanning probe methods are limited to surface structures, and the electron microscope can provide atomic resolution images of projections of crystalline materials in thicknesses up to about 50nm, or tomography of macromolecular assemblies and inorganics at lower resolution. No technique at present can provide three-dimensional imaging at nanometer resolution of the interior of particles in the micron size range. Coherent X-ray Diffractive Imaging (CXRD) is a way to provide this capability. Three ideas, developed over half a century, have now converged to provide a working solution to the non-crystallographic phase problem. We outline some applications and our development of this solution, which provides a method for lensless, diffractionlimited, aberration-free X-ray imaging of nano-objects in three-dimensions at high resolution. A CXDI experiment consists of three steps: (a) the sample is illuminated by monochromatic coherent x-rays and a recording is made of a single diffraction pattern (for 2D) or a tilt series (for 3D); (b) the phases of the pattern are recovered from the measured intensities using established phase-retrieval algorithms; (c) the unknown object is then recovered by Fourier inversion. In the Gerchberg-Saxton-Fienup scheme one starts with random phases, which lead to noise when transformed from reciprocal to real space. One then imposes the “finite support” constraint (namely that there must be a blank frame around the specimen), before transforming back to reciprocal space. In reciprocal space the phases so generated are combined with the measured diffraction magnitudes to start the next iteration. After a large number of iterations, in most cases the object emerges from the noise. Our novel improvement is that the estimate for the object support is continually updated by thresholding the intensity of the current object reconstruction. We start from a threshold of the transform of the diffraction pattern and as the iterations progress the support converges to a tight boundary around the object. This, in turn, improves the image reconstruction, which gives a better estimate of the support.

Our experiments in coherent diffraction began with trials using electron and visible-light optics and continued with CXDI at the Advanced Light Source (ALS). The experiments used the "pink" beam at beam-line 9.0.1 which is fed by a 10-cm-period undulator operating in third harmonic with deflection parameter (*K*) equal to 1.2 and delivering 588 eV (2.11 nm) photons. Features of the beam line include a 0.5 μm-thick, 750 μm-square Be window to separate the UHV beam line from the low-vacuum sample environment, a monochromator consisting of an off-axis segment of a zone plate and the diffraction experiment itself.

We have carried out three series of experiments, all using test samples made from 50 nm gold balls. The first demonstrated the basic 2D technique with image reconstruction using a support function determined by scanning electron microscopy. The second used a sample intentionally prepared in two separated parts, and reconstruction was achieved using information from the 2D diffraction pattern alone. The third series used a miniature sample rotation device to collect several tomographic data sets.A set of 150 views with at least a 100 second exposure time per view required about 10 hours. The 3D data generated are still being analysed.



Comparison of reconstructed soft X-ray image (middle) and SEM images of gold ball clusters (left). Each ball has a diameter of 50 nm

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